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Performance studies of the two-step multiboson algorithm in compact lattice QED *

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The performance of the two-step multiboson (TSMB) algorithm is investigated in comparison with the hybrid Monte Carlo (HMC) method for compact lattice QED with standard Wilson fermions both in the Coulomb and confinement phases. The restriction to QED allows for extensive measurements of autocorrelation times. Preliminary results show that the TSMB algorithm is at least competitive with standard HMC.

Compact lattice 4D QED with $N_f = 2$ dynamical Wilson fermions has been numerically studied [1] by means of the HMC algorithm [2]. However, the use of this algorithm within the confinement phase in the chiral limit $\kappa \to \kappa_c(\beta)$ as well as in the strong coupling phase with $\kappa > \kappa_c$ (the so-called 'Aoki phase') becomes cumbersome [3] because of large average condition numbers

$$\zeta = \frac{\langle \lambda_{\max} \rangle}{\langle \lambda_{\min} \rangle}. \qquad (1)$$

Here $\langle \lambda_{\max} \rangle$ and $\langle \lambda_{\min} \rangle$, respectively, are the largest and smallest average eigenvalues of the even-odd preconditioned Wilson fermion matrix $\mathcal{M}^\dagger \mathcal{M}$. Another open principal problem for the HMC method is the simulation of an odd number of fermion flavours. Hence, an alternative to the HMC method is desired. The same arguments hold also for lattice QCD and related models.

An alternative is provided by the hermitian two-step multiboson (TSMB) algorithm invented recently by one of the present authors (I.M.) [4]. It consists of the following basic ingredients. First, a polynomial approximation of the inverse fermion determinant [5] is introduced. Second, in order to reduce the computational costs [6–9] a noisy correction accept-reject step is employed. At the end one performs an auxiliary reweighting step for correcting the measured observables.

The TSMB algorithm has been successfully applied to a supersymmetric model [4]. Here we would like to investigate the efficiency of this algorithm in comparison with the standard HMC one. For this aim compact lattice QED with Wilson fermions provides a valuable test ground, because its fermionic properties - in particular in the confinement phase close to the chiral limit - resemble very much those of lattice QCD with Wilson fermions [3]. In this paper we consider always the case $N_f = 2$.

First of all, we want to establish a strategy for appropriately choosing the technical parameters for both the HMC and the TSMB algorithms. In order to achieve a reasonable acceptance rate for HMC we adjust the number of time steps N_τ and the time step size $\Delta\tau$ in the Hamilton dynamics according to the rule [10]

$$N_\tau \propto (\zeta^{1/4} \Delta\tau)^{-1}, \qquad \Delta\tau \propto (V\zeta)^{-1/4}, \qquad (2)$$

where ζ is defined in (1), and $V = N_s^3 \times N_4$ denotes the lattice volume. The stopping criteria for the conjugate gradient (CG) invertor in the Hamilton dynamics $\delta_{\rm HD}$ and for the accept-reject step $\delta_{\rm acc}$ are fixed in accordance with [11]

$$\delta_{\rm HD} \propto 1/V, \qquad \delta_{\rm acc} \propto 1/V^2\,. \qquad (3)$$

As a consequence the average number of CG iterations can be estimated to

$$\langle N^{(\rm CG)} \rangle \propto \zeta^{1/2} \ln V\,. \qquad (4)$$

The TSMB algorithm uses polynomials within the least squares integral approximation of the function $x^{-N_f/2}$ over the interval $[\epsilon, \lambda]$ (see [4,

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12]). The first (crude) polynomial of order n_1 is used in the first multiboson step. The second (correcting) polynomial of order n_2 is required for the noisy correction step. The third polynomial of order n_3 approximates the inverse square root of the second polynomial. And the fourth (finest) polynomial of the order n_4 is necessary for the reweighting step. These parameters are chosen according to a prescription in [13]:

$$n_1 \propto (\sqrt{\zeta})^{1/2} \ln V, \qquad n_2 \simeq \langle N^{(\mathrm{CG})} \rangle, \tag{5}$$

$$n_3 \simeq (1.2 \text{—} 1.4) n_2, \qquad n_4 \geq n_2, \tag{6}$$

$$\lambda \simeq (1.2 \text{—} 1.4) \langle \lambda_{\max} \rangle, \qquad \epsilon \simeq 0.5 \langle \lambda_{\min} \rangle. \tag{7}$$

For n_1 we have taken into account the empirical observation [12] that the dependence on the condition number becomes effectively weaker for the least squares first polynomial compared with polynomials in the Chebyshev approximation resulting in a replacement $\zeta \to \sqrt{\zeta}$.

Now let us come to the theoretical cost analysis. We define the performance of an algorithm by

$$\mathbf{P} = \mathbf{N}_{\mathrm{oper}} \tau_{\mathrm{int}}, \tag{8}$$

where $\mathbf{N}_{\mathrm{oper}}$ is the total number of operations per update. τ_{int} denotes the integrated autocorrelation time for a given observable. The numbers of operations in the HMC and in the TSMB ($n_2 \gg n_1$) algorithms are given as follows

$$\mathbf{N}_{\mathrm{oper}}^{\mathrm{HMC}} \propto V \langle N^{(\mathrm{CG})} \rangle N_\tau, \qquad \mathbf{N}_{\mathrm{oper}}^{\mathrm{TSMB}} \propto V n_2. \tag{9}$$

For simplicity instead of the value $\mathbf{N}_{\mathrm{oper}}$ we used the CPU time required for one sweep t_{CPU}. The integrated autocorrelation times for the HMC and the TSMB methods can be estimated according to arguments given in [10] and [6,8,9]

$$\tau_{\mathrm{int}}^{\mathrm{HMC}} \propto (N_\tau \Delta\tau)^{-2}, \quad \tau_{\mathrm{int}}^{\mathrm{TSMB}} \propto n_1 (\sqrt{\zeta})^{1/2}. \tag{10}$$

Here the effective dependence on the condition number ζ (1) for the least squares first polynomial has been taken into account, too. Thus, the expected theoretical gain $\mathbf{G}$ of the TSMB algorithm over the HMC method is evaluated according to (2), (4), (5), (8–10) as follows

$$\mathbf{G} \equiv \frac{\mathbf{P}^{\mathrm{HMC}}}{\mathbf{P}^{\mathrm{TSMB}}} \propto \frac{V^{1/4}}{\ln V}. \tag{11}$$

phase	N_τ	$\Delta\tau$	$\langle N^{(\mathrm{CG})} \rangle$
Coulomb	40	0.025	36.0(2)
confinement	10	0.01	500(2)

Table 1
HMC parameters for Coulomb and confinement phases. Stopping criteria are $\delta_{\mathrm{HD}} = 10^{-3}$ and $\delta_{\mathrm{acc}} = 10^{-7}$.

	n_1	n_2	n_3	n_4	ϵ	λ
(a)	6	36	48	200	0.025	2.5
(b)	50	360	450	500	0.000225	9

Table 2
TSMB parameters for Coulomb (a) and confinement (b) phases.

Now we turn to the numerical investigation of the performance of HMC and TSMB algorithms both in the Coulomb and confinement phases. The lattice size is $6^3 \times 12$ and time-antiperiodic boundary conditions for fermions are employed. In the Coulomb phase we have chosen the point $(\beta, \kappa) = (2.0, 0.130)$, whereas in the confinement phase $(\beta, \kappa) = (0.0, 0.238)$ quite close to the chiral limit. For the HMC method the number of time steps N_τ and the time step size $\Delta\tau$ selected according to the prescription (2) are presented in Table 1. The stopping criteria for the CG method according to (3) provide an average number of CG inversion steps (in the Hamiltonian dynamics) $\langle N^{(\mathrm{CG})} \rangle$ as shown in the same Table. In case of the TSMB algorithm the polynomial parameters are chosen according to the recipe (5–7) and presented in Table 2. The knowledge of these parameters requires information about the smallest $\langle \lambda_{\min} \rangle$ and largest $\langle \lambda_{\max} \rangle$ average eigenvalues of the even-odd preconditioned fermion matrix $\mathcal{M}^\dagger \mathcal{M}$, tunable to the dynamical fermion case from the quenched one (see Table 3).

The performance of the dynamical fermion algorithms was studied with respect to the average values of the following gauge invariant observables $\mathcal{O}$: the mean gauge plaquette energy

	quenched		dynamical	
	$\langle\lambda_{\rm min}\rangle$	$\langle\lambda_{\rm max}\rangle$	$\langle\lambda_{\rm min}\rangle$	$\langle\lambda_{\rm max}\rangle$
(a)	.065(1)	1.60(1)	.13(1)	1.63(1)
(b)	.0010(1)	6.78(1)	.0005(1)	6.59(1)

Table 3
Minimal $\langle\lambda_{\rm min}\rangle$ and maximal $\langle\lambda_{\rm max}\rangle$ average eigenvalue of the even-odd preconditioned Wilson fermion matrix $\mathcal{M}^\dagger\mathcal{M}$ for both Coulomb (a) and confinement (b) phases in quenched and dynamical cases, the latter determined from HMC.

	$\langle E_G\rangle$	$\langle\overline{\psi}\psi\rangle$	$\langle\Pi\rangle$
	Coulomb		
$\langle\mathcal{O}^{\rm HMC}\rangle$	0.1332(1)	0.9381(1)	1.378(1)
$\langle\mathcal{O}^{\rm TSMB}\rangle$	0.1331(1)	0.9379(1)	1.376(1)
$\tau_{\rm int}^{\rm HMC}$	3.2(3)	2.0(2)	25(4)
$\tau_{\rm int}^{\rm TSMB}$	3.0(3)	2.8(2)	50(8)
$\mathbf{G}$	1.7(2)	1.2(2)	0.8(2)
	Confinement		
$\langle\mathcal{O}^{\rm HMC}\rangle$	0.939(1)	0.95(1)	13.9(2)
$\langle\mathcal{O}^{\rm TSMB}\rangle$	0.938(1)	0.96(1)	13.7(2)
$\tau_{\rm int}^{\rm HMC}$	65(7)	60(7)	35(5)
$\tau_{\rm int}^{\rm TSMB}$	120(20)	125(15)	45(5)
$\mathbf{G}$	0.5(1)	0.5(1)	0.7(1)

Table 4
Performance of HMC and TSMB algorithms in the Coulomb and confinement phases.

$\langle E_G\rangle = \langle 1 - {\rm Re}\,U_{\rm p}\rangle$ the scalar condensate $\langle\overline{\psi}\psi\rangle$ and the pion norm $\langle\Pi\rangle = \langle(\overline{\psi}\gamma_5\psi)^2\rangle$. We measured the corresponding integrated autocorrelation times $\tau_{\rm int}$ and also the gain $\mathbf{G}$ (11) of the TSMB over the HMC method.

The main result of our investigation is presented in Table 4. The statistics in our case ($O(10^4)$ measurements) was sufficient to evaluate the integrated autocorrelation time. The reweighting procedure in the TSMB case has not changed significantly the results obtained using only the main two steps. We may conclude that the performance of the two algorithms is comparable for the chosen parameters. Further optimization of TSMB is possible by increasing the number of local gauge updates from one (in our case) to a larger number proportional to $\tau_{\rm int}^{\rm TSMB}$ in (10). Moreover, the polynomial degrees n_1 and n_2 could be taken smaller leaving more space for error correction by reweighting. This shows that for an even number of fermion flavours the TSMB algorithm is at least competitive with HMC.

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REFERENCES

1. A. Hoferichter, V. Mitrjushkin, M. Müller-Preussker, T. Neuhaus and H. Stüben, Nucl. Phys. B434 (1995) 358.
2. S. Duane, A. Kennedy, B. Pendleton and D. Roweth, Phys. Lett. B195 (1987) 216.
3. A. Hoferichter, V. Mitrjushkin, M. Müller-Preussker and H. Stüben, Phys. Rev. D58 (1998) 114505.
4. I. Montvay, Nucl. Phys. B466 (1996) 259.
5. M. Lüscher, Nucl. Phys. B418 (1994) 637.
6. M. Peardon (UKQCD Collaboration), Nucl. Phys. (Proc. Suppl.) B42 (1995) 891.
7. A. Borici and Ph. de Forcrand, Nucl. Phys. B454 (1995) 645.
8. K. Jansen, Nucl. Phys. (Proc. Suppl.) B53 (1997) 127.
9. A. Borici, hep-lat/9602018.
10. R. Edwards, I. Horvath and A. Kennedy, Nucl. Phys. B484 (1997) 375.
11. R. Gupta, G. Kilcup and S. Sharpe, Phys. Rev. D38 (1988) 1278.
12. I. Montvay, Comput. Phys. Commun. 109 (1998) 144.
13. S. Hands, I. Montvay, S. Morrison, M. Oevers, L. Scorzato and J. Skullerud, Eur. Phys. J. C17 (2000) 285.